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6. AUTHORS
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14. ABSTRACT
Collective electron excitations in quasi-1D/2D systems such as pristine and hybrid carbon nanotubes (CNs), crossed semiconductor nanowires, and planar graphitic structures, are studied theoretically using rigorous methods of quantum electrodynamics, in order to identify new physical effects of relevance to future applications in advanced nanomaterials engineering. For pristine semiconducting CNs, optically excited excitons are demonstrated to be able to amplify interband plasmons. Strong local coherent fields produced in this way can be used for near-field sensing,

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Report Title

Final Report: New Concepts for the Development of Carbon Nanotube Materials for Army Related Applications

ABSTRACT

Collective electron excitations in quasi-1D/2D systems such as pristine and hybrid carbon nanotubes (CNs), crossed semiconductor nanowires, and planar graphitic structures, are studied theoretically using rigorous methods of quantum electrodynamics, in order to identify new physical effects of relevance to future applications in advanced nanomaterials engineering. For pristine semiconducting CNs, optically excited excitons are demonstrated to be able to amplify interband plasmons. Strong local coherent fields produced in this way can be used for near-field sensing, energy conversion, and materials nanoscale modification. We also predict the effect of the exciton Bose-Einstein condensation in individual semiconducting CNs. This opens up new horizons for CN based applications ranging from tunable highly coherent polarized light source to the extension of nanoplasmonics research to include a new area of CN plasmonics. For hybrid CN systems consisting of a pair of spatially separated extrinsic atoms, ions, molecules, or quantum dots that are physisorbed on the CN surface, we give recommendations on how to control time evolution of bipartite atomic entanglement in such systems by using strong laser pulses. Such systems are of interest to quantum information science. We also study the Casimir interaction in graphitic nanostructures such as double wall CNs, single layer and bilayer graphene. Overlapping interband plasmon resonances from both tubes are shown to be responsible for stronger inter-tube attraction in double wall CN systems. Graphene optical transparency is demonstrated to be the main reason for the reduced inter-layer graphene attraction as compared to that of perfect metals. Properly chosen materials for substrates and fluid can induce a Casimir repulsion for graphene flakes suspended in a fluid between substrates. Finally, an easy-to-use program code for the Wolfram Mathematica package is developed that is precise enough to simulate dynamical excitonic dielectric response functions for individual CNs with diameters greater than one nanometer.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
08/06/2014	27.00	I. V. Bondarev, A. V. Meliksetyan. Possibility for exciton Bose-Einstein condensation in carbon nanotubes, Physical Review B, (04 2014): 1. doi: 10.1103/PhysRevB.89.045414
08/06/2014	28.00	M. F. Gelin, I. V. Bondarev, A. V. Meliksetyan. Optically promoted bipartite atomic entanglement in hybrid metallic carbon nanotube systems, The Journal of Chemical Physics, (02 2014): 1. doi: 10.1063/1.4863971
08/16/2015	54.00	Tobias Hertel, University of Wuerzburg, Germany, Igor Bondarev, NC Central University, USA. Photophysics of carbon nanotubes and nanotube composites, Chemical Physics, (02 2013): 0. doi: 10.1016/j.chemphys.2012.12.010
08/27/2013	18.00	Anh D. Phan, Lilia M. Woods, D. Drosdoff, I. V. Bondarev, N. A. Viet. Temperature dependent graphene suspension due to thermal Casimir interaction, Applied Physics Letters, (07 2012): 113118. doi: 10.1063/1.4752745
08/27/2013	21.00	M.F. Gelin, I.V. Bondarev, A.V. Meliksetyan. Monitoring bipartite entanglement in hybrid carbon nanotube systems via optical 2D photon-echo spectroscopy, Chemical Physics, (02 2013): 123. doi: 10.1016/j.chemphys.2012.09.027
08/27/2013	19.00	I V Bondarev, M F Gelin, W Domcke. Plasmon nanooptics with individual single wall carbon nanotubes, Journal of Physics: Conference Series, (11 2012): 1. doi: 10.1088/1742-6596/393/1/012024
08/27/2013	17.00	D. Drosdoff, A. D. Phan, L. M. Woods, I. V. Bondarev, J. F. Dobson. Effects of spatial dispersion on the Casimir force between graphene sheets, The European Physical Journal B, (11 2012): 1. doi: 10.1140/epjb/e2012-30741-6
08/28/2012	7.00	I. V. Bondarev, T. Antonijevic. Surface plasmon amplification under controlled exciton-plasmon coupling in individual carbon nanotubes, physica status solidi (c), (05 2012): 1259. doi: 10.1002/pssc.201100125
08/28/2012	8.00	I. Bondarev. Single-wall carbon nanotubes as coherent plasmon generators, Physical Review B, (01 2012): 35448. doi: 10.1103/PhysRevB.85.035448
08/28/2012	9.00	I. V. Bondarev, L. M. Woods, A. Popescu. On the role of interband surface plasmons in carbon nanotubes, Optics and Spectroscopy, (12 2011): 733. doi: 10.1134/S0030400X11120046

TOTAL: 10

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

(1.) Subash Chandra Nepal, "Binding Energy of Quantum Bound States in X-shaped Nanowire Intersection" (Prof. I.V.Bondarev, thesis advisor)
A thesis in partial fulfillment of the requirements for the degree of Master of Science in Physics, North Carolina Central University, Durham, North Carolina, 2014

(2.) Liubov Zhemchuzhna, "Bound electron states in skew-symmetric quantum wire intersections" (Prof. I.V.Bondarev, thesis advisor)
A thesis in partial fulfillment of the requirements for the degree of Master of Science in Physics, North Carolina Central University, Durham, North Carolina, 2014

Number of Presentations: 2.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received		Paper
08/07/2014	33.00	I.V.Bondarev,, A.V.Meliksetyan. Possibility for exciton Bose-Einstein condensation in carbon nanotubes, APS March Meeting 2014, Denver, CO, USA. 03-MAR-14, . : ,
08/07/2014	34.00	S. Nepal, , L. Zhemchuzhna, , A. V. Meliksetyan, , I. V. Bondarev. Bound electronstates in skew-symmetric quantum wire intersections, APS March Meeting 2014 . 03-MAR-14, . : ,
08/07/2014	35.00	I.V.Bondarev,, A.V.Meliksetyan. Binding energy of the trion complex in carbon nanotubes, APS March Meeting 2014, Denver, CO, USA. 03-MAR-14, . : ,
08/07/2014	36.00	I.V.Bondarev,, A.V.Meliksetyan. Exciton-plasmon interaction effects and optical properties of individual carbon nanotubes, Optics of Excitons in Confined Systems (OECS13) Rome, Italy. 09-SEP-13, . : ,
08/07/2014	37.00	I. V. Bondarev, , M. F. Gelin, , A. V. Meliksetyan, , L. M.Woods. Near-field plasmonic effects in carbon nanotubes, Diamond and Carbon Materials (DCM2013), Riva del Garda, Italy. 02-SEP-13, . : ,
08/16/2015	40.00	I.V.Bondarev , M.F.Gelin,, A.V.Meliksetyan. Tunable near-field plasmonic effectsin individual carbon nanotubes, 14th International Conference on the Science and Application of Nanotubes (NT13, June 24–28, 2013, Helsinki, Finland). 24-JUN-13, . : ,
08/16/2015	52.00	D. Drosdoff, L.M. Woods, A. Phan, I.V. Bondarev, N. Viet. Temperature-dependent levitation of a graphene flake due to Casimir forces, APS March Meeting, March 18–22, 2013, Baltimore, MD, USA. 18-MAR-13, . : ,
08/16/2015	51.00	I.V. Bondarev. Asymptotic exchange coupling of quasi-one-dimensional excitons in carbon nanotubes, 7th International Symposium on Computational Challenges and Tools for Nanotubes (CCTN11 – NT11 satellite, July 15–16, 2011, Cambridge, UK). 15-JUL-11, . : ,
08/16/2015	50.00	I.V. Bondarev, T. Antonijevic. Plasmon generation by optically excited excitons in individual single wall carbon nanotubes, 12th International Conference on the Science and Application of Nanotubes (NT11, July 10–14, 2011, Cambridge, UK). 10-JUL-11, . : ,
08/16/2015	49.00	I.V.Bondarev. Nanotube plasmonics, International Conference "Spins & Photonic Beams at Interface" (September 25-27, Minsk, Belarus). 25-SEP-11, . : ,
08/16/2015	48.00	I.V. Bondarev, M.F. Gelin, W. Domcke. Plasmon nanooptics with pristine and hybrid nanotube systems, APS March Meeting, February 27–March 2, 2012, Boston, MA, USA. 27-FEB-12, . : ,
08/16/2015	47.00	I.V. Bondarev, M.F. Gelin, W. Domcke. Plasmon nanooptics with pristine and hybrid carbon nanotube systems, International Conference ”Dubna-Nano 2012” (July 9–14, 2012, Dubna, Russia).. 09-JUL-12, . : ,

08/16/2015	53.00	A.V. Meliksetyan, I.V. Bondarev, A.V. Chizhov, M.F. Gelin. Quantum optics effects in hybrid metallic carbon nanotube systems, 5th International Workshop on nanotube optics and nanospectroscopy (WONTON13, June 16–20, 2013, Santa Fe, NM, USA). 16-JUN-13, . : ,
08/16/2015	45.00	A.V. Meliksetyan, I.V. Bondarev, M.F. Gelin. Non-linear optical response simulations for strongly corellated hybrid carbon nanotube systems, APS March Meeting, March 18–22, 2013, Baltimore, MD, USA. 18-MAR-13, . : ,
08/16/2015	44.00	I.V.Bondarev, A.V.Meliksetyan. Exciton-plasmon interaction effects in individual carbon nanotubes, APS March Meeting, March 18–22, 2013, Baltimore, MD, USA. 18-MAR-13, . : ,
08/16/2015	43.00	I.V.Bondarev, M.F.Gelin, A.V.Meliksetyan. Tunable Near-Field Plasmonic Effects in Individual Carbon Nanotubes, 6th International Conference on surface plasmons photonics (SPP6, May 26–31, 2013, Ottawa, Canada).. 26-MAY-13, . : ,
08/16/2015	42.00	I.V.Bondarev, A.V.Meliksetyan. Properties of Exciton-Plasmons in Individual Carbon Nanotubes, 5th International Workshop on nanotube optics and nanospectroscopy (WONTON13, June 16–20, 2013, Santa Fe, NM, USA) . 16-JUN-13, . : ,
08/31/2012	11.00	I.V.Bondarev, T. Antonijevic. Plasmon generation by excitons in carbon nanotubes, Proceedings of the Nanotech 2012 Conference. 18-JUN-12, . : ,

TOTAL: **18**

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received		Paper
08/27/2013	25.00	M.F. Gelin, I.V. Bondarev, A.V. Meliksetyan. Optically-promoted bipartite atomic entanglement in hybrid metallic carbon nanotube systems, Journal of Physical Chemistry C (07 2013)
08/27/2013	26.00	I.V. Bondarev, A.V. Meliksetyan. Possibility for exciton Bose-Einstein condensation in carbon nanotubes, Physical Review Letters (05 2013)
08/28/2012	1.00	A. D. Phan, L. M. Woods, D. Drosdoff, I. V. Bondarev, J. F. Dobson. Effects of spatial dispersion on the Casimir force between graphene sheets, Europhysics Letters (05 2012)
08/28/2012	2.00	A. D. Phan, L. M. Woods, D. Drosdoff, I. V. Bondarev, N. A. Viet. Temperature dependent graphene suspension due to thermal Casimir interaction, Applied Physics Letters (08 2012)
08/28/2012	3.00	I. V. Bondarev, M. F. Gelin, W. Domcke. Plasmon nanooptics with individual single wall carbon nanotubes, Journal of Physics: Conference Series (08 2012)
08/28/2012	5.00	M. F. Gelin, I. V. Bondarev, A. V. Meliksetyan. Monitoring bipartite entanglement in hybrid carbon nanotube systems via optical 2D photon-echo spectroscopy, Chemical Physics (06 2012)

TOTAL: **6**

Number of Manuscripts:

Books

Received	Book

TOTAL:

Received	Book Chapter
08/16/2015 39.00	I.V. Bondarev, M.F. Gelin, A.V. Meliksetyan. Tunable Plasmon Nano-Optics with Carbon Nanotubes, New York, USA: CRC Press, Taylor & Francis Group, (03 2014)
08/27/2013 20.00	I.V. Bondarev, M.F. Gelin, A.V. Meliksetyan. Tunable Plasmon Nano-Optics with Carbon Nanotubes, Dekker Encyclopedia of Nanoscience and Nanotechnology: Taylor & Francis, (03 2013)
TOTAL:	2

Patents Submitted

A. Popescu, L.M. Woods, and I.V. Bondarev, "Carbon nanotube oscillator surface profiling device and method of use"

Patents Awarded

A. Popescu, L.M. Woods, and I.V. Bondarev, "Carbon nanotube oscillator surface profiling device and method of use", US Patent No 8,060,943 (issued on November 15, 2011); Assignees: University of South Florida (Tampa, FL), North Carolina Central University (Durham, NC)

Awards

(1.)☼ The University of North Carolina Research Opportunities Initiative (ROI) Award, 2015: project title — ”NC carbon materials initiative: Materials design, processing, and manufacturing for defense and energy needs”; period — 03/2015–06/2017; Partnering institutions — NC State University, NC Central University, UNC-Chapel Hill; Theory Support PI — Igor Bondarev, NCCU ($140,872 of total award funding $2,829,994; Lead PI — Harald Ade, NCSU)

(2.) The US Department of Energy, Office of Basic Energy Sciences, 2014: award No DE-SC0007117 (extended); project title — ”Near-field electrodynamics of carbon nanostructures”; period — 09/2014–08/2017; amount — $300,000

(3.) North Carolina Central University, USA, 2014: Faculty Senate certificate of appreciation in recognition of service (academic year 2013-14)

(4.) The US National Science Foundation, 2013: award No ECCS-1306871; project title — ”QMHP: Tunable plasmon nanooptics with carbon nanotubes”; period — 09/2013–08/2016; amount — $291,900

(5.)☼ North Carolina Central University, USA, 2013: Faculty Senate certificate of appreciation in recognition of service (academic year 2012-13)

(6.)☼ North Carolina Central University, USA, 2012: College of Science and Technology Excellence in Research Award

(7.)☼ North Carolina Central University, USA, 2012: Office of Sponsored Research Award for Research and Technology Innovations

(8.)☼ The US Department of Energy, Office of Basic Energy Sciences, 2011: award No DE-SC0007117; project title—” Surface electromagnetic phenomena in pristine and atomically doped carbon nanotubes: Fundamentals and applications”; period — 09/2011–08/2014; amount — $300,000

(9.)☼ NT2011 — 12th International Conference on the Science and Application of Nanotubes: award certificate for outstanding contribution to the satellite symposium on Computational Tools and Challenges for Nanotubes (CCTN2011)

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Subash Nepal	1.00	
Liubov Zhemchuzhna	1.00	
Oluwafemi Adelegan	1.00	
Clement Etukakpan	1.00	
Esan Israel	1.00	
Mawufemor Kudadze	0.85	
Frederick Aryeetey	0.85	
Brandon Davis	0.30	
FTE Equivalent:	**7.00**	
Total Number:	**8**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Dr. Areg Meliksetyan	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Dr. Igor Bondarev	0.17	
Dr. Kinney Kim	1.00	
FTE Equivalent:	**1.17**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Daniel Rasic	0.50	Physics
FTE Equivalent:	**0.50**	
Total Number:	**1**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 1.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 1.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 1.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 1.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 1.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 1.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 1.00

Names of Personnel receiving masters degrees

NAME	
Subash Nepal	
Liubov Zhemchuzhna	
Clement Etukakpan	
Oluwafemi Adelegan	
Esan Israel	
Mawufemor Kudadze	
Frederick Aryeetey	
Brandon Davis	
Total Number:	8

Names of personnel receiving PHDs

NAME	
Total Number:	

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

5 **Carbon nanotube oscillator surface profiling device and method of use**

Patent Filed in US? (5d-1) Y
Patent Filed in Foreign Countries? (5d-2) N
Was the assignment forwarded to the contracting officer? (5e) N
Foreign Countries of application (5g-2):

5a: Igor Bondarev

5f-1a: North Carolina Central University

5f-c: 1801 Fayetteville Str
Durham NC 27707

5a: Lilia Woods

5f-1a: University of South Florida

5f-c: 4202 E. Fowler Avenue
Tampa FL 33620

5a: Adrian Popescu

5f-1a: University of South Florida

5f-c: 4202 E. Fowler Avenue
Tampa FL 33620

Scientific Progress

See Attachment

Technology Transfer

n/a

SUMMARY OF RESEARCH ACCOMPLISHMENTS (2011-15)

Localized (trapped) and delocalized low-energy collective electron excitations in quasi-one/two-dimensional (1D/2D) systems, such as pristine and hybrid carbon nanotubes, crossed semiconductor nanowires, and planar graphitic structures, have been studied theoretically using rigorous methods of quantum mechanics and quantum electrodynamics, in order to identify new physical effects of relevance to future generation applications in nanomaterials engineering.

(1) We demonstrate for the first time a possibility for the exciton Bose-Einstein condensation in individual small-diameter (∼1–2 nm) semiconducting carbon nanotubes (CNs). The effect occurs under the exciton-interband-plasmon coupling controlled by an external electrostatic field applied perpendicular to the nanotube axis. The effect requires fields ∼1 V/nm and temperatures below 100 K that are experimentally accessible. The quantum system we study is conceptually similar to the microcavity exciton-polariton system, which started as a theoretical concept in the 1990s and has been a driving force for experimental physics of low-dimensional semiconductors over the last two decades, exhibiting both new fundamental quantum effects and attractive applications such as polariton lasers, optical polarization switches, superfluid spintronic devices, etc. We, therefore, strongly believe that the quasi-1D exciton BEC effect we predict not only offers a testing ground for fundamentals of condensed matter physics in one dimension, but also opens up new horizons for a variety of CN based applications ranging from controlled electromagnetic absorption and tunable highly coherent polarized light emission, in particular, to the extension of nanoplasmonics and near-field optics research, currently focused mostly on metallic nanoparticles, to include a new area of nanotube plasmonics. **[Fig. 1; <u>I.V.Bondarev and A.V.Meliksetyan, Physical Review B 89, 045414 (2014)</u>]**

(2) Optically excited excitons are theoretically demonstrated to generate and amplify surface plasmons in individual semiconducting carbon nanotubes. Surface plasmons are coherent charge density waves due to the periodic opposite-phase displacements of the electron shells with respect to the ion cores. Charge density waves produce oscillating electric fields concentrated locally throughout the nanotube surface. The entire process can be controlled by a perpendicular electrostatic field. Our theoretical research shows that the non-radiative exciton-to-plasmon energy transfer, whereby the external electromagnetic radiation absorbed to excite excitons transfers into the energy of surface plasmons, can efficiently mediate and greatly enhance the electromagnetic absorption by pristine semiconducting nanotubes. This enhancement is caused by the buildup of the macroscopic population numbers of coherent localized surface plasmons producing high-intensity local oscillating fields throughout the nanotube surface. The strong local coherent fields produced in this way can be used in various new technological applications of carbon nanotubes, such as near-field sensing, optical switching, electromagnetic energy conversion, and materials nanoscale modification. **[Fig 2; <u>I.V.Bondarev, Physical Review B 85, 035448 (2012)</u>]**

(3) We study theoretically a pair of spatially separated extrinsic atomic type species (extrinsic atoms, ions, molecules, or semiconductor quantum dots) near a metallic carbon nanotube, that are coupled both directly via the inter-atomic dipole-dipole interactions and indirectly by means of the virtual exchange by resonance plasmon excitations on the nanotube surface. We analyze how the optical preparation of the system by using strong laser pulses affects the formation and evolution of the bipartite atomic entanglement. Despite a large number of possible excitation regimes and evolution pathways, we find a few generic scenarios for the bipartite entanglement evolution. We formulate practical recommendations on how to control the robust bipartite atomic entanglement in hybrid CN systems. **[Fig. 3; collaborative work with Advanced Photonics Center at Munich Technical University, Germany; <u>M.F.Gelin, I.V.Bondarev, and A.V.Meliksetyan, The Journal of Chemical Physics 140, 064301 (2014)</u>]**

(4) We analyze the angular dependence of the lowest energy bound state for an electron trapped at the intersection of two identical semiconductor nanowires crossed at an arbitrary angle. When the nanowires are perpendicular, such a classically unbound system is known to possess a

quantum bound state [R.L.Schult, et al, PRB 39, 5476 (1989)]. We use the variational approach to study how the binding energy of the lowest bound state varies as a function of the wire intersection angle. Using two different trial wave functions, we simulate two intersection types, X-type and S-type, different in their respective channel intersection areas (diamond for the former and square for the latter). For both geometries, the binding energy generally decreases as the intersection angle deviates from the right angle. The S-type wire intersection preserves the bound state even at angles close to zero degree, as opposed to the X-type intersection. Our data supplement a theory of quantum bound states in classically unbound systems and may be useful to interpret electron transport peculiarities in realistic systems such as semiconductor nanowire films and carbon nanotube bundles. **[<u>S.Nepal, L.Zhemchuzhna, A.V.Meliksetyan, and I.V.Bondarev, Bulletin of the American Physical Society, Vol. 59, No 1, p. H1.00147</u> (APS March Meeting, March 3–7, 2014, Denver, CO, USA); also: <u>MS Thesis by S.Nepal and MS Thesis by L.Zhemchuzhna, NCCU-2014 (I.V.Bondarev, thesis advisor)</u>]**

(5) We employ a unified macroscopic quantum electrodynamics approach to study the Casimir interaction in graphitic nanostructures of different geometry configurations, such as carbon nanotubes, single layer and bilayer graphene. At the quantum mechanical limit (T = 0 K), it is found by direct calculations of single-nanotube electron energy loss spectra that the nanotube/nanotube interaction in a double wall CN system is profoundly affected by the collective low-energy (interband) plasmon excitations of individual constituent nanotubes. It is shown that pronounced, low-energy peaks in the CN electron energy loss spectra are a main factor contributing to the strength of the inter-tube attraction. The overlap of the low-energy inter-band plasmon resonances in both tubes warrant stronger inter-tube attraction and better stability of the double wall CN system. The graphene/graphene Casimir force is also investigated. It is obtained that the graphene optical transparency is the main reason for the reduced inter-layer graphene attraction as compared to the one for perfect metals. We also propose that at finite temperatures the thermal Casimir force effect can be observed for a graphene flake suspended in a fluid between substrates. Properly chosen materials for the substrates and fluid can even induce a Casimir repulsion. The balance with other forces, such as gravity and buoyancy, results in a stable temperature dependent equilibrium separation of the graphene flakes in the suspension. Suspended graphene is thus a promising system for observing the thermal Casimir force effects at room temperatures. **[Fig.4; collaborative work with University of South Florida (USF) @ Tampa; <u>L.M.Woods, A.Popescu, D.Drosdoff, and I.V.Bondarev, Chemical Physics 413, 123 (2013); A.D.Phan, L.M.Woods, D.Drosdoff, I.V.Bondarev, and N.A.Viet, Applied Physics Letters 101, 113118 (2012)</u>]**

(6) An easy-to-use, low-time-consuming program code for the Wolfram Mathematica package has been developed that is precise enough to simulate dynamical excitonic dielectric response functions and axial surface conductivities for individual semiconducting and metallic carbon nanotubes with diameters greater than one nanometer. The conventional $k{\cdot}p$ scheme for semiconductor band-structure calculations is used within the screened Hartree-Fock approximation. An efficient numerical algorithm is implemented to diagonalize the matrix eigenvalue problem with the electron-hole Coulomb interaction in the momentum space, in order to obtain exciton excitation energies and wave functions for dark and bright excitonic states in carbon nanotubes. Results are compared with density-functional-theory (DFT) simulations. In the low-energy region ~0.5–1.5 eV of main interest to us, our calculations agree quantitatively within one percent with those reported by the DFT method for the exciton excitation energies in carbon nanotubes with diameters greater than one nanometer. Also, an efficient Mathematica code has been developed for simulations of the local (distance dependent) density of photonic states (DOS) responsible for the non-radiative decay of excited atomic type species (modeled by a two-level dipole emitter) due to their interaction with nanotube's photonic modes in the near-field zone when nearby the CN surface. Thus, we are able to simulate quantitatively the non-radiative decay and other near-field interaction processes for atomic type species and excitons in the presence of metallic and semiconducting CNs. **[Examples of calculations shown in Fig. 5 (a) & (b)]**

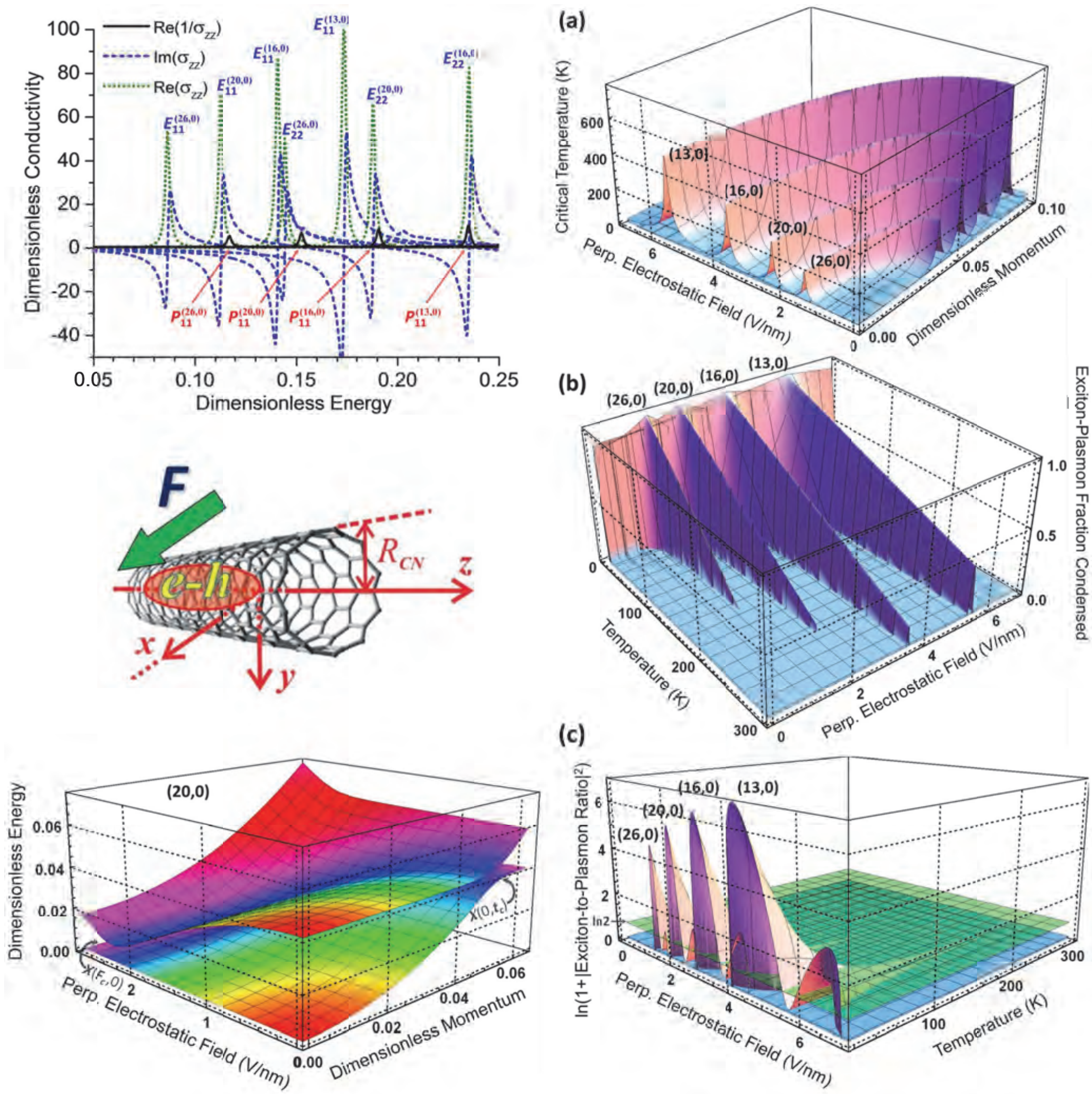

Figure 1. *Top left*: Calculated energy dependences of the axial surface conductivity σ_{zz} for the four semiconducting CNs, (13,0), (16,0), (20,0) and (26,0), of increasing diameters. Peaks of Reσ_{zz} and of Re$(1/\sigma_{zz})$ represent excitons (E_{11}, E_{22}) and inter-band plasmons (P_{11}, P_{22}), respectively. Dimensionless energy is defined as [*Energy*]/$2\gamma_0$, where γ_0 = 2.7 eV is the C-C overlap integral. *Left, middle and bottom*: The geometry of the problem and the exciton-plasmon dispersion for the lowest bright exciton coupled to the nearest inter-band plasmon in the (20,0) CN [$E_{11}^{(20,0)}$ and $P_{11}^{(20,0)}$ in top left]. *Right, top to bottom*: Critical BEC temperatures (a), mean exciton-plasmon BEC population (b) and the exciton contribution (c) to the exciton-plasmon BEC population, for the four CNs under consideration.

I.V.Bondarev and A.V.Meliksetyan, Phys. Rev. B 89, 045414 (2014)

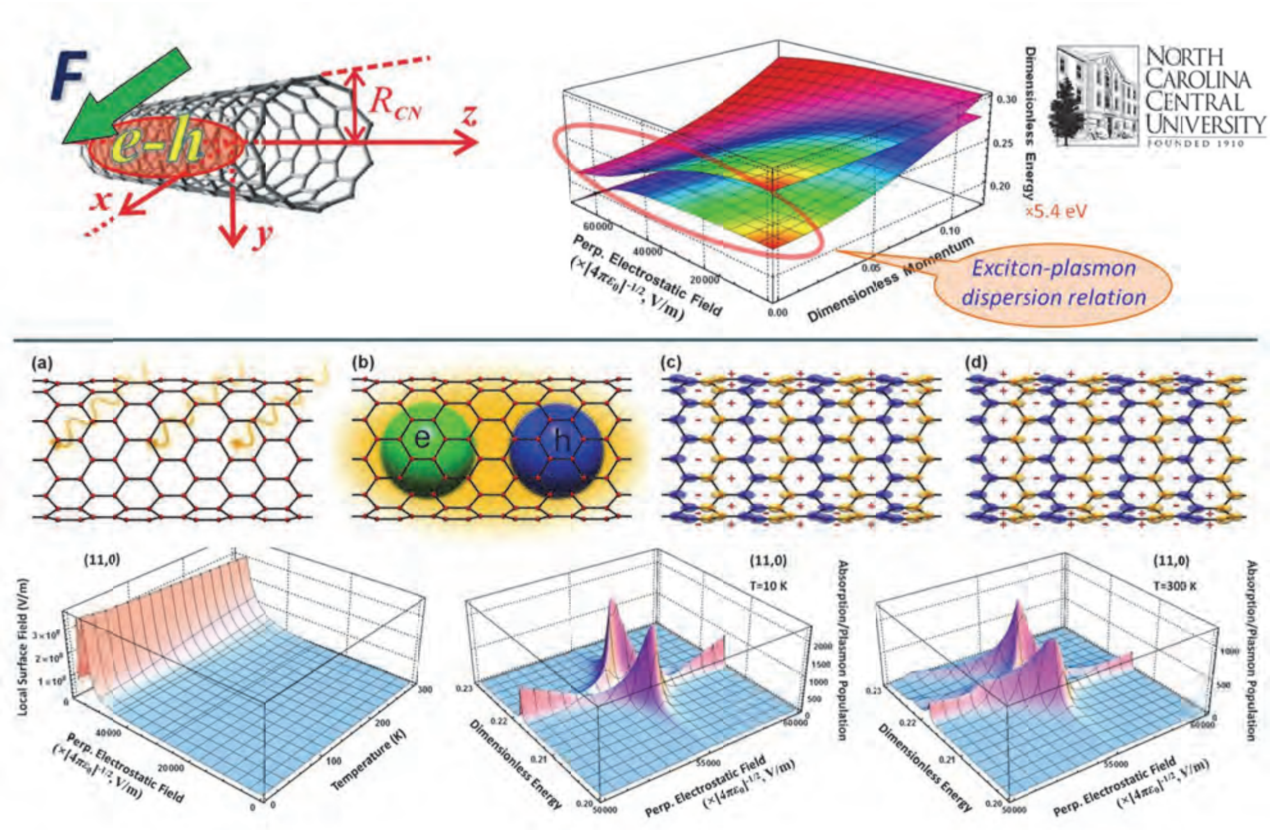

Figure 2. *Top row*: Exciton-plasmon dispersion relation (right) as a function of a perpendicular electrostatic field applied (left) and longitudinal momentum for the 1st bright exciton in the (11,0) nanotube. *Middle row, left to right*: Schematic of the plasmon generation process by the optically excited exciton. (a),(b) Exciton excitation by the external electromagnetic radiation. (c),(d) Plasma oscillations (produced by the non-radiative exciton decay) are periodic opposite-phase displacements of the electron shells relative to the ion cores in the neighboring elementary cells (blue and yellow) of the nanotube. Such periodic displacements induce coherent oscillating electric fields (shown by + and − signs) of zero mean magnitude, but non-zero mean-square magnitude, concentrated locally across the nanotube diameter throughout the nanotube length. *Bottom row, left*: Local surface field amplitude as a function of temperature and perpendicular electrostatic field applied; *Bottom row, middle and right*: Low-*T* and high-*T* plasmon population (also representing increased light absorption by excitons). All calculations are done for the 1st bright exciton in the (11,0) CN.

I.V.Bondarev, Phys. Rev. B 85, 035448 (2012)

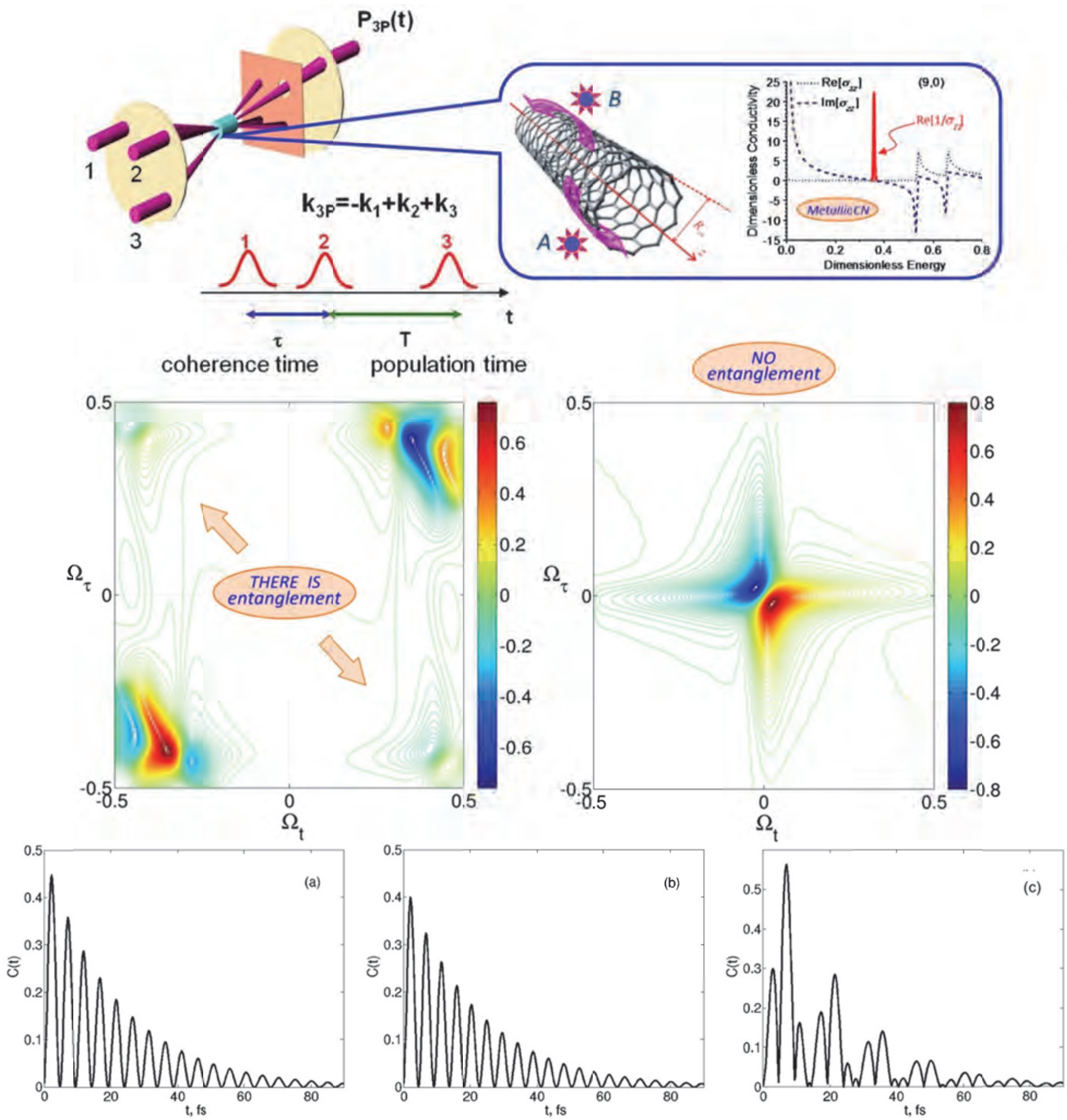

Figure 3. *Top and middle*: Schematic of the optical 2D photon-echo spectroscopy experiment and calculated representative 2D spectra for the bipartite entanglement monitoring of the two spatially separated two-level dipole emitters, two-level systems (TLS) *A* and *B* (which may be a pair of atoms, ions, or quantum dots), coupled to the same plasmon resonance of a metallic CN (inset on top). *Bottom row*: Calculated time evolution of the bipartite concurrence (representative of entanglement) for equal TLS-CN coupling constants $\mu_A = \mu_B = 0.3$ eV and counter-phase initial *A* and *B* population amplitude preparation with zero (a) and non-zero [=0.3 eV] (b) inter-TLS dipole-dipole coupling constant; (c) same as in (b) for $\mu_A = 0.3$ eV and $\mu_B = 0.1$ eV.

M.F.Gelin, I.V.Bondarev & A.V.Meliksetyan, J. Chem. Phys. 140, 064301 (2014)
Chem. Phys. 413, 123 (2013)

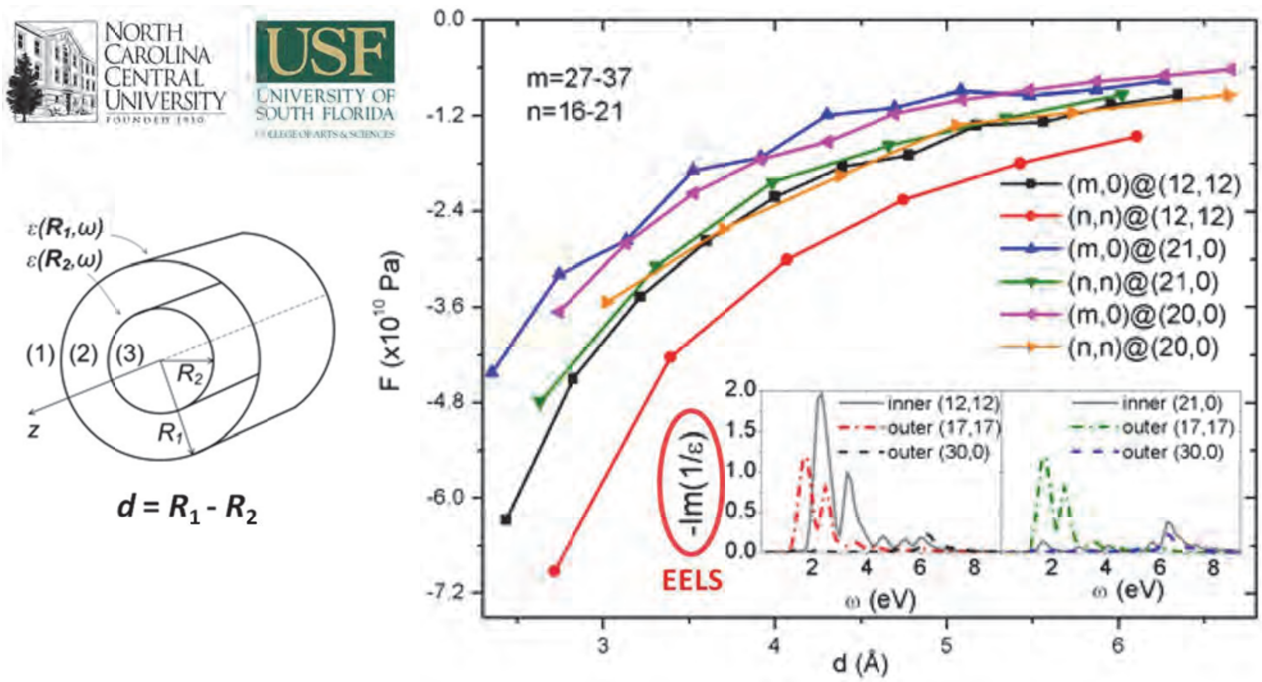

Figure 4: Calculated Casimir forces versus inter-tube separation distance for various double wall carbon nanotube combinations. The existence of strong overlapping interband plasmon resonances (see the inset) in double wall nanotube combinations with both inner and outer tubes being metallic results in their stronger attraction and better stability as a consequence. This study presents a unified quantum approach we have developed and used for vacuum-type electromagnetic interactions in graphitic nanostructures, which is able to consistently take into account both their unique electronic response properties and particular geometry configurations. More examples of our calculations and new results can be found in the following publiucations.

L.M.Woods, A.Popescu, D.Drosdoff & I.V.Bondarev, Chem. Phys. 413, 123 (2013)
A.D.Phan, L.M.Woods, D.Drosdoff, I.V.Bondarev & N.A.Viet, Appl. Phys. Lett. 101, 113118 (2012)
D.Drosdoff, A.D.Phan, L.M.Woods, I.V. Bondarev & J.F.Dobson, Eur. Phys. J. B 85, 365 (2012)
A.Popescu,L.M.Woods & I.V.Bondarev, Phys. Rev. B 83, 081406(R) (2011)

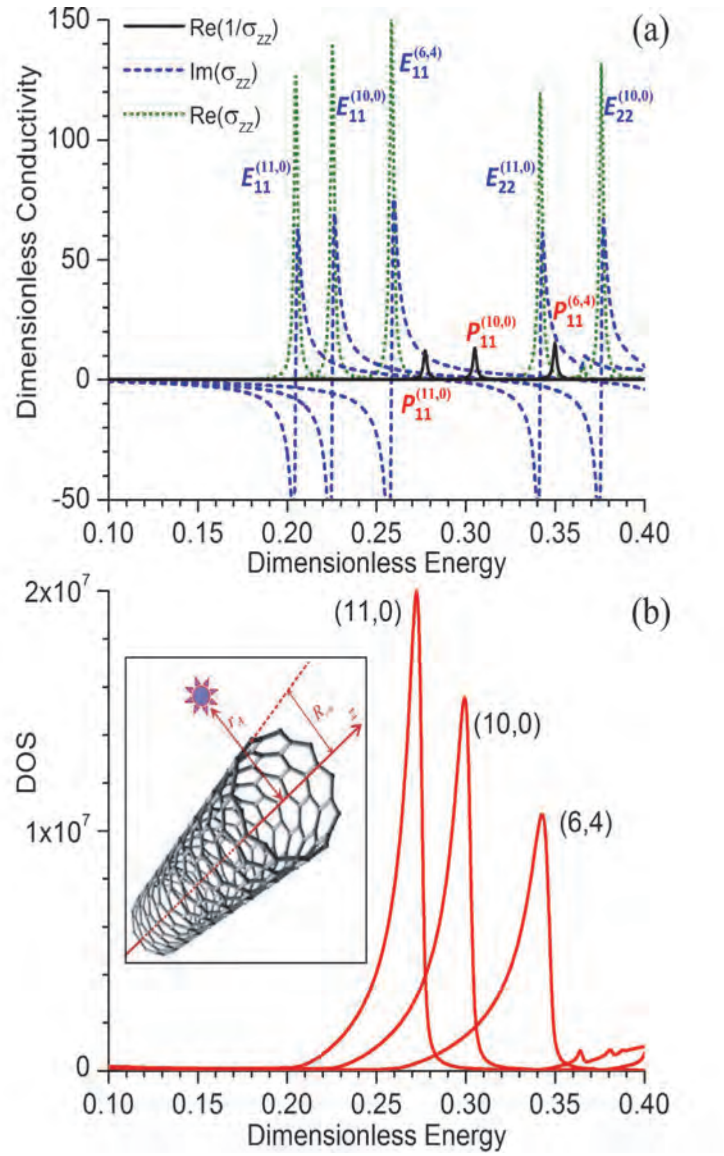

Figure 5.

(a) Fragment of the calculated energy dependences of the dimensionless axial surface conductivities σ_{zz} (normalized by $e^2/2\pi\hbar$) for the semiconducting (6,4), (10,0) and (11,0) carbon nanotubes of increasing diameter. Peaks of Re(σ_{zz}) represent excitons (E_{11}, E_{22}, ...); peaks of Re($1/\sigma_{zz}$) represent inter-band plasmons (P_{11}, ...). Dimensionless energy is defined as [*Energy*]/$2\gamma_0$ with $\gamma_0 = 2.7$ eV being the carbon-carbon nearest-neighbor overlap integral.

(b) Photonic DOS functions calculated for the CNs in (a) with the two-level dipole emitter at the distance $r_A = R_{CN} + 2b$ (R_{CN} is the CN radius, b =1.42 Å is the carbon-carbon nearest neighbor distance) from the CN symmetry axis (see inset). Sharp single-peak resonances originating from the inter-band plasmon modes of the respective nanotubes [cf. (a) and (b)], are responsible for the TLS-CN interaction in the near-field zone.

PUBLICATIONS IN WHICH ARO SUPPORT IS ACKNOWLEDGED (2011-15)

A. Journal Publications

(1.) I.V. Bondarev and A.V. Meliksetyan, "Possibility for exciton Bose-Einstein condensation in carbon nanotubes",
Physical Review B, Vol. 89, p. 045414, 2014

(2.) M.F. Gelin, I.V. Bondarev, and A.V. Meliksetyan, "Optically promoted bipartite entanglement in hybrid metallic carbon nanotube systems",
The Journal of Chemical Physics, Vol. 140, p. 064301, 2014

(3.) T. Hertel and I.V. Bondarev, "Editorial: Photophysics of carbon nanotubes and nanotube composites",
Chemical Physics, Vol. 413, p. 1, 2013

(4.) M.F. Gelin, I.V. Bondarev, and A.V. Meliksetyan, "Monitoring bipartite entanglement in hybrid carbon nanotube systems via optical 2D photon-echo spectroscopy",
Chemical Physics, Vol. 413, p. 123, 2013

(5.) A.D. Phan, L.M. Woods, D. Drosdoff, I.V. Bondarev, and N.A. Viet, "Temperature dependent graphene suspension due to thermal Casimir interaction",
Applied Physics Letters, Vol. 101, p. 113118, 2012

(6.) I.V. Bondarev, M.F. Gelin, and W. Domcke, "Plasmon nanooptics with individual single wall carbon nanotubes",
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(7.) D. Drosdoff, A.D. Phan, L.M. Woods, I.V. Bondarev, and J.F. Dobson, "Effects of spatial dispersion on the Casimir force between graphene sheets",
The European Physical Journal B, Vol. 85, p. 365, 2012

(8.) I.V. Bondarev and T. Antonijevic, "Surface plasmon amplification under controlled exciton-plasmon coupling in individual carbon nanotubes",
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(9.) I.V. Bondarev, "Single wall carbon nanotubes as coherent plasmon generators",
Physical Review B, Vol. 85, p. 035448, 2012 (selected for the February 13, 2012 issue of the Virtual Journal of Nanoscale Science & Technology at http://www.vjnano.org)

(10.) I.V. Bondarev, L. M. Woods, and A. Popescu, "On the role of interband surface plasmons in carbon nanotubes",
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B. Books or Other Non-Periodical, One-Time Professional Publications

(11.) I.V. Bondarev, M.F. Gelin, and A.V. Meliksetyan, "Tunable plasmon nanooptics with carbon nanotubes",
In: Dekker Encyclopedia of Nanoscience and Nanotechnology, 3rd ed., CRC Press: New York, 2014, pp. 4989-5001

(12.) I.V. Bondarev and A.V. Meliksetyan, "Possibility for exciton Bose-Einstein condensation in carbon nanotubes",
In: Bulletin of the American Physical Society, Vol. 59, No 1, p. Y37.00002 (APS March Meeting, March 3–7, 2014, Denver, CO, USA)

(13.) S. Nepal, L. Zhemchuzhna, A.V. Meliksetyan, and I.V. Bondarev, "Bound electron states in skew-symmetric quantum wire intersections",

In: Bulletin of the American Physical Society, Vol. 59, No 1, p. H1.00147 (APS March Meeting, March 3–7, 2014, Denver, CO, USA)

(14.) A.V. Meliksetyan and I.V. Bondarev, "Binding energy of the trion complex in carbon nanotubes",
In: Bulletin of the American Physical Society, Vol. 59, No 1, p. Y37.00005 (APS March Meeting, March 3–7, 2014, Denver, CO, USA)

(15.) I.V. Bondarev and A.V. Meliksetyan, "Exciton-plasmon interaction effects and optical properties of individual carbon nanotubes",
In: 13th International Conference on Optics of Excitons in Confined Systems (OECS13, September 9–13, 2013, Rome, Italy). Book of abstracts, p. 214

(16.) I.V. Bondarev, M.F. Gelin, A.V. Meliksetyan, and L.M.Woods, "Near-field plasmonic effects in carbon nanotubes",
In: International Conference on Diamond and Carbon Materials (DCM2013, September 2–5, 2013, Riva del Garda, Italy). Book of abstracts, p. O.052

(17.) I.V. Bondarev, M.F. Gelin, and A.V. Meliksetyan, "Tunable near-field plasmonic effects in individual carbon nanotubes",
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(18.) I.V. Bondarev and A.V. Meliksetyan, "Possibilities for Bose-Einstein condensation in individual carbon nanotubes",
In: 8th International Symposium on Computational Challenges and Tools for Nanotubes (CCTN13 – NT13 satellite, June 29, 2013, Tallinn, Estonia). Book of abstracts, p. 244

(19.) I.V. Bondarev, A.V. Chizhov, M.F. Gelin, and A.V. Meliksetyan, "Quantum optics effects in hybrid metallic carbon nanotube systems",
In: 5th International Workshop on nanotube optics and nanospectroscopy (WONTON13, June 16–20, 2013, Santa Fe, NM, USA). Book of abstracts, p. P17

(20.) I.V. Bondarev and A.V. Meliksetyan, "Properties of exciton-plasmons in individual carbon nanotubes",
In: 5th International Workshop on nanotube optics and nanospectroscopy (WONTON13, June 16–20, 2013, Santa Fe, NM, USA). Book of abstracts, p. P18

(21.) I.V. Bondarev, M.F. Gelin, and A.V. Meliksetyan, "Tunable near-field plasmonic effects in individual carbon nanotubes",
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(22.) I.V. Bondarev and A.V. Meliksetyan, "Exciton-plasmon interaction effects in individual carbon nanotubes",
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(23.) A.V. Meliksetyan, I.V. Bondarev, and M.F. Gelin, "Non-linear optical response simulations for strongly corellated hybrid carbon nanotube systems",
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(24.) A. Phan, D. Drosdoff, L.M. Woods, I.V. Bondarev, N. Viet, "Temperature-dependent levitation of a graphene flake due to Casimir forces",
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(25.) I.V. Bondarev, M.F. Gelin, and A.V. Meliksetyan, "Tunable plasmon nanooptics with carbon nanotubes",

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(26.) I.V. Bondarev, M.F. Gelin, and W. Domcke, "Plasmon nanooptics with pristine and hybrid carbon nanotube systems",
In: International Conference ”Dubna-Nano 2012” (July 9–14, 2012, Dubna, Russia). Book of abstracts, p. 29

(27.) I.V. Bondarev and T. Antonijevic, "Plasmon generation by excitons in carbon nanotubes",
In: Proceedings of the Nanotech 2012 Conference (June 18–21, 2012, Santa Clara, CA, USA), Vol.1, p.334

(28.) I.V. Bondarev, M.F. Gelin, and W. Domcke, "Plasmon nanooptics with pristine and hybrid nanotube systems",
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(29.) I.V. Bondarev, "Nanotube plasmonics",
In: International Conference ”Spins & Photonics Beams at Interface” (September 25–26, 2011, Minsk, Belarus). Book of abstracts, p. 9

(30.) I.V. Bondarev and T. Antonijevic, "Plasmon generation by optically excited excitons in individual single wall carbon nanotubes",
In: 12th International Conference on the Science and Application of Nanotubes (NT11, July 10–14, 2011, Cambridge, UK). Book of abstracts, #121

(31.) I.V. Bondarev, "Asymptotic exchange coupling of quasi-one-dimensional excitons in carbon nanotubes",
In: 7th International Symposium on Computational Challenges and Tools for Nanotubes (CCTN11 – NT11 satellite, July 15–16, 2011, Cambridge, UK). Book of abstracts, #122

C. Patents

(32.) A. Popescu, L.M. Woods, and I.V. Bondarev, "Carbon nanotube oscillator surface profiling device and method of use",
US Patent No 8,060,943 (issued on November 15, 2011); Assignees: University of South Florida (Tampa, FL), North Carolina Central University (Durham, NC)

D. Student Master Theses Completed

(33.) Subash Chandra Nepal, "Binding Energy of Quantum Bound States in X-shaped Nanowire Intersection" (Prof. I.V.Bondarev, thesis advisor)
A thesis in partial fulfillment of the requirements for the degree of Master of Science in Physics, North Carolina Central University, Durham, North Carolina, 2014

(34.) Liubov Zhemchuzhna, "Bound electron states in skew-symmetric quantum wire intersections" (Prof. I.V.Bondarev, thesis advisor)
A thesis in partial fulfillment of the requirements for the degree of Master of Science in Physics, North Carolina Central University, Durham, North Carolina, 2014